Markov Property Applications to Ising Model Calculations

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Abstract The Markov property is described. Its application to parallel computation and the potential for computational speed-up from its use are illustrated in both exact and Monte Carlo computations for the one and two dimensional, near-neighbor Ising models.

1. Introduction

First let me remind the reader what the Markov property referred to in the title is. Suppose that you have a problem defined on some (metric) space. Draw a boundary which separates the space into an "inside" and an "outside." If the system has the Markov property, then if we fix the problem variables on the boundary, then any quantity "inside" is completely independent of the "outside." For example, in a spin-$\frac{1}{2}$, nearest-neighbor Ising model, the problem would be a (large) portion of a regular space lattice (like the simple-cubic lattice, for example). The problem space can then be separated by fixing the spins on a boundary that leaves no inside-spin with any outside-spin as a nearest neighbor. The Markov property follows for this case because the partition function factors as

$$Z = Z(\text{inside} + \text{boundary})Z(\text{outside} + \text{boundary}). \tag{1}$$

This Markov property is a key property which allows the dissection of the problem into may parallel problems. It is appropriate for massively parallel computation. The point of this presentation is to begin to find ways to exploit this insight.

2. Exact Calculations

One way that I have found to use this property is in making advances in exact computation. The area of application is the Ising model on the two-dimensional, plane-square lattice. For this model we have an exact analytic solution [1] for the partition function, the energy and the specific heat, but there are many other quantities of interest for which there is no known analytic solution. Examples are the magnetic susceptibility, its second derivative and the correlation length. From these quantities we may construct a key quantity in the modern, renormalization group theory of critical phenomena, the renormalized coupling constant, g^*, which is defined by

$$g(K) = -\frac{v}{a^d}\frac{\frac{\partial^2 \chi}{\partial H^2}}{\chi^2 \xi^d},$$
$$g* = \lim_{K \to K_c} g(K), \tag{2}$$

where v is the volume of a unit cell, a is the lattice spacing, d is the spatial dimension, H is the magnetic field, χ is the magnetic susceptibility, ξ is the correlation length, and K is the exchange energy J over Boltzmann's constant times the temperature. In this work we will use the second moment definition for the correlation length and implement it by means of the limit $|\vec{k}| \to 0$ of

$$\xi^2(\vec{k}) = \frac{1}{4\sum_{l=1}^{d} \sin^2(\frac{1}{2}k_l a)} \left(1 - \frac{\chi(N, \vec{k}, K)}{\chi(N, \vec{0}, K)}\right), \tag{3}$$

where N is the system edge length in lattice spacings and

$$\chi(N, \vec{k}, K) = \frac{1}{N}\langle \left| \sum_{\vec{\jmath}=\vec{1},\vec{N}} \exp(ia\vec{k}\cdot\vec{\jmath})\sigma_{\vec{\jmath}} \right|^2 \rangle, \tag{4}$$

with $\langle\ \rangle$ denoting the expectation value with respect to the sum over all the spin states with the usual Gibbs weight, and the sum over $\vec{\jmath}$ denoting the sum over all lattice sites.

I have found that, of the possible compact shapes, the diamond seems to be the most efficient for the plane square lattice, in the sense that it has the lowest boundary to total number of spins ratio. The most primitive such diamond is just the four nearest neighbors of a single spin. If we denote these nearest-neighbor spins as σ_a, where $a = n, e, s, w$ in reference to the four directions, then the partition function is

$$Z_2(K) = 2\cosh(K(\sigma_n + \sigma_e + \sigma_s + \sigma_w)), \tag{5}$$

Table 1. Renormalized Coupling Constant

N	g^*
2	1.8253
4	2.2339
6	2.4505
8	2.5556
10	2.6152
∞	2.676

where the sum over the central spin has been carried out. Expressions can easily be given for $\langle(\frac{1}{4}(\sigma_n + \sigma_e + \sigma_s + \sigma_w) + \sigma_c)^n\rangle_{\mathcal{B}}$ where the subscript $\mathcal{B}$ means the four boundary spins are held fixed. With this result, we can put four 2×2 diamonds together and sum them over the one central spin to get a 3×3 diamond as a function of the states of its 8 boundary spins. Repeating this process with 3×3 diamonds we can create a 5×5 diamond of 41 spins and 20 boundary spins by summing over the 5 new interior spins. Other such procedures can lead to the construction of the 4×4 and 6×6 diamonds, *etc.* By use of periodic boundary conditions, it is straightforward to paste two $2n \times 2n$ diamonds together to form one $4n - 2 \times 4n - 2$ square with periodic boundary conditions. I have done this for 2×2 to 10×10 squares, and computed the renormalized coupling constant for these cases. Since $\xi^2 \propto K$ for small K, it is most convenient to discuss $\hat{g} = Kg(K)/K_c$ where $K_c = \text{arctanh}(\sqrt{2} - 1)$ is the critical point for this model. Series [2] and theoretical [3] analysis indicates that for the infinite system size limit, $\hat{g}(K)$ increases smoothly from $\hat{g}(0) = 2/K_c$ to about $\hat{g}(K_c) = 14.5 \pm 0.2$. Our exact results form a monotonically increasing sequence (lying below the $N = \infty$ case). They all have peaks and the location of the peak increases towards K_c as N increases. It is interesting to note that while Ferdinand and Fisher [4] found that the difference between the peak location and K_c for the specific heat is $K_c - K_{\text{peak}} \approx 0.35/N$, we find that for these relatively small N values it moves very slowly towards K_c. The representation $K_c - K_{\text{peak}} \propto 1/\sqrt{N}$ conveys a sense of the peak behavior. Another interesting feature is reported in Table 1. The values of $g(K_c)$ as a function of N increase very slowly, and do not in the least appear to be converging to the expected value of 14.5, but rather a crude extrapolation suggests a value closer to 2.7. This observation coupled with the slow rate of convergence of the peak to K_c suggests that $\lim_{N\to\infty} g(K)$ is a discontinuous function of K. It is well known that the limit of a sequence of continuous functions can be a discontinuous function if they are not uniformly continuous, however it makes the work considerably harder to extract correctly the limit, $\lim_{K\to K_c} \lim_{N\to\infty}$, which is the physically desired result.

3. Monte Carlo Calculations

To apply the Markov property to a Monte Carlo calculation of the two dimensional Ising model, first divide the lattice into diamonds of a uniform size. Then pick one diamond and label it A. Going along a horizontal row label the rest of the diamonds B and A alternately. Then beginning with this labeled row proceed vertically and label every diamond A and B alternately in each vertical column through a labeled diamond. This procedure will label half the diamonds but every diamond border spin will lie on exactly one labeled diamond if we agree not to associate the spins with either the east or south diamond vertices. With a table of the results for the small diamonds one can then do a Monte Carlo simulation on the boundary spins of the A diamonds, *in parallel*, and then on the B diamonds, also *in parallel*. The use of these pre-tabulated results for the small diamonds effectively incorporates much of the computation necessary for the exact results in parallel into the Monte Carlo computation. By the factorization properties of the partition function, to compute the probability of flipping a boundary spin we need to compute the product only of the two diamonds (four for a boundary vertex) that have the spin on their boundary. This product is need for the current spin state and for the flipped spin state. If the diamonds are called I and II, then the spin flip probability is,

$$\text{flip probability} = \frac{W_{\rm I}(\text{flip})W_{\rm II}(\text{flip})}{W_{\rm I}(\text{flip})W_{\rm II}(\text{flip}) + W_{\rm I}(\text{current})W_{\rm II}(\text{current})}, \qquad (6)$$

for a Metropolis type algorithm where W_a is the weight for the diamond a. Early results indicate that the auto-correlation time is given by

$$\tau_D \approx A_D \xi^{z_D}, \qquad (7)$$

where D is the size of the diamond, and A_D decreases strongly and z_D decreases slightly as D increases.

In the case of the Ising model in one dimension, a study [5] has been done. Here the process is the same. The subunits are line segements of length $m+2$, with the center m spins summed out. Here because of the simplicity of the problem, the necessary results can be computed analytically or, of course, also numerically. The results in this case is the mapping of the original Ising model on to a new Ising modlel of fewer spins and at a higher temperature. The partition function maps as

$$Z(K) = \sum_{\{\sigma_i = \pm 1\},\ i=1,\ldots,N} \exp\left(K \sum_i \sigma_i \sigma_{i+1} \right) \mapsto$$

$$Z(K_m) \propto \sum_{\{\sigma_i = \pm 1\},\ i=1,m+1,2m+2,\ldots} \exp\left(K_m \sum_{i=1,m+1,\ldots} \sigma_i \sigma_{i+m+1} \right), \qquad (8)$$

where the mapped parameter is given by

$$\exp(K_m) = \frac{1 - \tanh^{m+1} K}{1 + \tanh^{m+1} K}. \qquad (9)$$

The autocorrelation time for the Metropolis algorithm for this model is

$$\tau = 1.00 \xi^{2.0} \qquad (10)$$

within about 5% . The dynamical critical exponent does not depend on m as can be seen from the mapping (8-9), in contrast to early indications for the two dimensional model mentioned above. The speed up factor on a machine like the CM 200 can be of the order of a million, and is given, asymptotically as the critical point is approached, by $N_p(m+1)^3 = N_p(m+1)^{1+z}$. Here N_p is the number of central processors; the factor $m+1$ comes because with the same machine resources there are fewer spins to do; and the factor $(1+m)^z$ comes from the decrease in the autocorrelation time because K_m is smaller than K due to (9). The provision of time on the CM-200 by the Los Alamos Advanced Computing Laboratory is gratefully acknowledged.

References

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